

Mini-symposium B12

Quantum Transport Modeling and Simulation for Atomic Scale Two-Dimensional Materials

Organizers:

Saroj K. Nayak
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Fri - 9 Jan 2015 | 11:00 – 12:30 | Room 04-33, Block S16

Chair: Saroj Nayak

11:00 B12-01 Keynote
Using Localized Orbitals to Describe Electronic Structure and Quantum Transport in Two-Dimensional Materials
Pablo Ordejón
ICN2 - Institut Català de Nanociència i Nanotecnologia, Campus UAB, 08193 Bellaterra, Barcelona (Spain)

11:30 B12-02 Invited
Electronic Transport in Polycrystalline Graphene and Monolayer Transition Metal Dichalcogenides
Oleg V. Yazyev
Institute of Theoretical Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

12:00 B12-03 Invited
Electronic transport, nanostructuring and disorder in graphene
Stephen R. Power, Mikkel Settnes, Søren Schou Gregersen, Thomas Aktor, Antti-Pekka Jauho
Center for Nanostructured Graphene (CNG), Department of Micro- and Nanotechnology (DTU Nanotech), Technical University of Denmark.

Fri - 9 Jan 2015 | 14:00 – 15:30 | Room 04-33, Block S16

Chair: Vitor M Pereira

14:00 B12-04 Invited
PN-junctions in graphene: focusing and snake states
Francois PEETERS
University of Antwerp, Department of Physics, Groenenborgerlaan 171, B-2020 Antwerpen

14:30 B12-05 Invited
User friendly quantum transport in magnetic graphene bars: Landauer @ non-collinear selfconsistent calculations
Jose Lado, Joaquin Fernandez-Rossier
International Iberian Nanotechnology Laboratory (INL), Braga, Portugal

15:00 B12-06
Large magnetoresistance from long-range interface coupling in armchair graphene nanoribbon junctions
Suchun Li, Young-Woo Son⁴, Su Ying Quek^{1,2}
¹*Department of Physics, National University of Singapore, Singapore,* ²*Institute of High Performance Computing, Agency for Science, Technology and Research, Singapore,* ³*NUS Graduate School for Integrative Sciences and Engineering, National University of Singapore, Singapore,* ⁴*Korea Institute for Advanced Study, Seoul 130-722, Korea*

15:15 B12-07
Low Resistance Metal Contacts to MoS2 Devices with Nickel-Graphene Electrodes
Xin Luo^{1,2}, Wei Sun Leong³, Khoong Hong Khoo^{1,2}, Yida Li³, John T. L. Thong³ and Su Ying Quek^{1,†}
¹*Department of physics, National university of Singapore,* ²*Institute of High Performance Computing,* ³*Department of electrical and computer engineering, National university of Singapore.*

Fri - 9 Jan 2015 | 16:00 – 17:30 | Room 04-33, Block S16

Chair: Vitor M Pereira

16:00 B12-08 Invited
Transport in Single and Multilayer Graphene: Polynomial Expansions on Video Cards
Lucian Covaci
Universiteit Antwerpen, Antwerpen, Belgium

16:30 B12-09 Invited
First-principles Study of the Electronic Structure and Phase Stability of Two-dimensional Hexagonal Hybrid Cx(BN)1-x Nanomaterials
Sugata Mukherjee¹, Ransell D'Souza²
¹*S.N. Bose National Centre for Basic Sciences Block JD, Sector III, Salt Lake, Kolkata 700098 India,* ²*S.N. Bose National Centre for Basic Sciences Block JD, Sector III, Salt Lake, Kolkata 700098 India*

17:00 B12-10
Influence of confined optical phonons on the Radioelectric effect in doping superlattice
Nguyen Quang Bau, Do Tuan Long
Faculty of Physics, Hanoi University of Science, Vietnam National University, 334-Nguyen Trai, Hanoi, Vietnam

17:15 B12-11
The quantum acoustomagnetolectric field in a doped superlattice GaAs:Si/GaAs:Bi in the presence of an external electromagnetic wave.
Nguyen Van Hieu¹, Le Hong Son¹, Nguyen Quang Bau², Nguyen Dinh Nam², Nguyen Van Hieu¹
¹*Department of physics, Danang University, No. 459 Ton Duc Thang Str., Hoa Khanh Dist., Danang, Vietnam,* ²*Department of Physics, College of Natural Sciences, Hanoi National University No. 334, Nguyen Trai Str., Thanh Xuan Dist., Hanoi, Vietnam.*